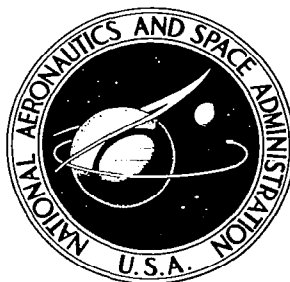


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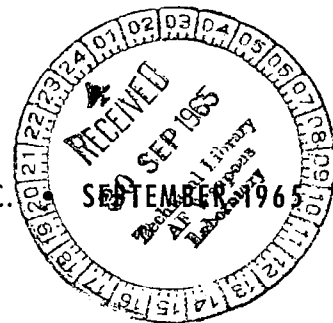
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IMPROVED DATA HANDLING TECHNIQUES FOR SPECTROMETER DATA

Prepared under Contract No. NAS 5-9087 by
DELTA DATA SYSTEMS, INC.
College Park, Md.

for

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION • WASHINGTON, D. C.





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ABSTRACT

A mathematical method to improve resolution and select solar emission lines in spectrometer data is presented. The method depends upon non-linear averaging, numerical band-pass filtering, and second differences. Spectra representing scans of the solar emission intensity from 40 to 400 Å are computed. Line intensities as low as 35 counts per second above background and separated by 0.4 Å or more are detected.

Computer programs for the GSFC direct coupled IBM 7050/7094 have been written to execute the algorithms developed and are presented.

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INTRODUCTION

Mathematical and numerical procedures have been developed which permit determination of intensity and position of emission lines with counting rate greater than or equal to thirty five (35) counts per second above background and separated from their nearest neighbors by 0.4 \AA or more. Confidence levels for the intensity and position have been established for the lines detected.

Computer programs have been written which perform the details of the computations. The results have been compiled and presented in listings and plots. The computer used in this effort was an IBM 7050-7094 system located at the Goddard Space Flight Center.

Four solar spectra representing selected periods of solar activity have been analyzed using the above-mentioned program. This step required the processing of approximately 200 scans of the solar spectrum (40A - 400A) selected by the technical officer. Each scan consisted of 2500 data pairs, a value for the counting rate and a value for the position of the Rowland circle. The data was recorded on magnetic tape in IBM Fortran II binary format. These tapes are in the digital tape library of the Solar Physics Branch of the Space Sciences Division at GSFC and were made available by the technical officer as required. A computer program for combining data into averages was also made available.

Working programs for all computations made are furnished. These include source decks, binary decks, definition of input-output variables, and complete instructions for preparing runs on the computer.

A document detailing and justifying the mathematical and numerical techniques used for the computations performed under this project has been prepared.

Four (4) plots have been prepared defining by position and amplitude each spectral line studied. The coordinate system used was log intensity (counts/sec) vs linear distance (cm) of the exit slit from the grating. The log scale covers three decades, from 10^1 to 10^4 , with eight inches for each decade. The horizontal position scale covered the scanning range of 4.25 - 23.4 cm along the Rowland circle with 6.25 inches for each cm of scan.

The prime experiment flown on the first Orbiting Solar Observatory was a soft x-ray spectrometer designed specifically to make satellite measurements of the solar spectrum from wavelengths of 10 to 400 Angstroms (Reference 1). As a result of the successful launch of the satellite into a near circular earth orbit, 550 km perigee and 600 km apogee, and the subsequent successful operation of the experiment, the first long term measurements of the soft x-ray solar spectrum were obtained.

The angular aperture of the spectrometer was approximately 1.2 by 2.2 degrees. Hence, with moderately accurate pointing (within plus or minus a few minutes of the center of the solar disc), the spectrometer responded to the total light intensity emitted by the sun. The orientation of the spectrometer was such that the sunlight fell perpendicularly on the front face of the instrument, passed through the entrance slit and struck a concave grating mounted in grazing incidence, the angle of incidence was 88 degrees. The diffracted rays continued to the exit slit in front of the detector. The detector was mounted on a carriage, which moved on

a circular rail so that the exit slit followed along the Rowland circle where the spectrum was in focus.

The detector used was an open window multiplier phototube developed by the Bendix Corporation specifically for use in this spectrometer and designated the M-306. The electrical pulses were amplified and after coding were recorded on a tape recorder for later transmission to a ground station.

Analysis of the data to determine the correct behavior of the spectrometer hardware during the experiment has indicated a drift of the markers, possibly due to marker wear. The influence of this wear on the data was compensated for by designing the computer program to follow the strong lines as references, i.e. to seek them out. Variations in motor speed which could cause localized distortions have been accounted for by selecting references which are just close enough to optimize the correction for this possible defect in the data, and yet not be so close that the errors in locating the references introduce significant fluctuations in the computation of scale factors for the nonlinear averaging process. The scale factors are included as part of the print-out during computation, thus further study of distortions is facilitated.

The post acquisition processing which has been applied to the data which is available for processing by the computer programs developed should be discussed. The voltage-analog data is digitized by counting transitions in telemetered voltage level and taking the sum at predetermined selected times to calculate the counting rate. The counting rate is a measure of the photons arriving at the photomultiplier which produce pulses. The photomultiplier efficiency is of the

order of 3%. The photons arriving at the photomultiplier are those which have passed through the entrance slit, have been focused by the concave grating and have passed through the slit at the photomultiplier.

The current is actually computed by

$$I = \frac{P}{\Delta t} = \frac{8N}{\alpha c}$$

where P is the number of photons counted. A binary counter is used on board the satellite and the telemetered voltage is changed when 8, 128, and 2048 photons have been counted. N is increased by 1 each time 8 photons are counted. A 2 kc. oscillator is used to drive the post processing hardware, call this the clock. This oscillator is retuned after every minute of satellite data has been processed. The number of cycles the oscillator has made is c in the expression for the counting rate. Thus, if $8/\alpha$ is a constant then the computed current is this constant multiplied by a rational fraction, N/c . Expect the counting rate to be quantized. Indeed, a table of all possible counting rates is easily computed. The algorithm used by the hardware to determine the counting rate is as follows: during processing count c, count N. When $c=21$ and as soon as N is increased again compute the counting rate or as soon as $N=16$ compute the counting rate.

Consider counting rates sufficiently high so that a class two transition $N=16$ is certain to occur before $c=21$. Label

t_s = clock cycle time in seconds and

t_D = Data time in seconds.

Further, define β as the number of clock cycles per Data time. Thus,

$$t_D = \beta t_s .$$

If the photon current is constant and such that β is not exactly integer then the rounded value of β , write β_R , will occasionally be one more or less than the normal value. Refer to these abnormal currents as "beat" currents. The normal current may then be written

$$I = \frac{P}{t_D} = \frac{P}{\beta t_s}$$

where P is the number of photons collected. Since the process of digitization must use β_R current values are calculated by

$$I = \frac{P}{\beta_R t_s}.$$

Under the assumption that the photon current is constant the sampling interval is constant, and the number of data intervals between "beat" current values is

$$n_D = 1/|\beta - \beta_R|$$

where β_R is the nearest integer to β . Also, the number of clock cycles between "beat" currents is

$$n_s = n_D \beta = \beta/|\beta - \beta_R|$$

The minimum n_s or maximum oscillation frequency is achieved for β half integer and is

$$n_s(\min) = 2\beta \text{ } (\beta \text{ half integer}).$$

n_s becomes increasingly large as β approaches integer values from either side.

It can be shown that if

$$\beta - \beta_R > 0 \quad \text{then } I_B < I_R$$

and if

$$\beta - \beta_R < 0 \quad \text{then } I_B > I_R$$

where I_B is the value of the "beat" current and I_R is the usual or regular output data value. Also note the true current I lies between I_R and I_B .

Invert n_s and obtain the frequency with which beat values are obtained per clock cycle as the unit of time. Thus,

$$\text{Frequency of Beats} = | \beta - \theta_R | / \theta.$$

This mathematical phenomenon clearly explains the oscillations at the peak of the Helium 304 line. It is suspected that this phenomenon is exhibited at very low wavelengths where the scattered light enhances the counting rate greatly.

MATHEMATICAL CONCEPTS

The progress of observational astrophysics depends in two ways upon supporting disciplines. First, there are experiments which in this case include spectrometers, supporting electronics, and a laboratory; in other words, the engineering aspects. The second dependence is in the area of presentation of results. Grain density in photoelectric emulsions contributes to the diffusion of information. Photodensitometer data and satellite telemetered data have received considerable attention with respect to the possibility of applying more sophisticated mathematical methods to objectively select information with increased resolution (Reference 9).

The signal as it leaves the environment of the sun could be considered a set of delta functions in the intensity wavelength coordinate system. The delta functions are thermally broadened, but this broadening is insignificant, being approximately $1/5000^{\text{th}}$ of the final diffused profile observed. The data arrives at the satellite environment essentially undisturbed. The atmosphere does produce some scattering which is significant only inside of the spectrometer. There is, of course, some absorption. Also, there is an additive signal detected when passing through the South Atlantic magnetic anomaly due to triggering by ionized particles.

The concave grating has the disadvantage that incident light is scattered forward strongly independent of wavelength. This produces an apparent strong signal at shorter wavelengths. The relationship governing the intensity of scattered light background is approximately given by

$$y = ax^{-b}$$

The entrance slit to the spectrometer appears at the focus point of the Rowland circle as a uniformly lit image. As the photoelectric detector which is mechanically transported along the Rowland circle crosses the focused image of the entrance slit, its own slit has the effect of diffusing the otherwise rectangular intensity into a triangular profile.

The photodetector with a yield of 3% and an approximate 50% variation now introduces the first significant noise into the data. If the scanning is slow, the noise is averaged out. If the scanning is rapid, the noise remains significant. During data acquisition the position of the detector on the Rowland circle is introduced as part of the data by permitting the travelling detector carriage to trip contact switches. The contact reliability is influenced by wear, dirt, carriage wobbling and contact aspect.

The assumption is that the signal now available is indeed a series of simple triangles, with amplitude noise, often superimposed to form composites or blends. The data yet in psuedo-analog format must now be digitized to permit the application of the mathematics developed here. The process of digitization due to the sampling rate used has the effect of integrating the analog signal over a portion of the spectrum which we might call the sampling interval. The average intensity and the central position for this interval are computed and presented as input data to the present effort. The assumption used that these data are points on a smooth function has the obvious effect of rounding the corners of the triangular profiles. It can be shown that if the sampling is equally spaced but in random phase with respect to the profile center that, with the a/d sampling rate used, the peak counting rate will probably be

reduced by 10%. Two effects of the finite sampling rate are, first, that each digitized data point is effectively rounded; secondly, counting rates representing high intensity portions of the spectrum, such as at the peak of the helium line demonstrate a mathematical phenomenon known as beating (page 5). The oscillator controlling the sampling during a/d conversion is retuned each minute which represents about 2.25 centimeters along the Rowland circle.

Variations in detector speed, due to variations in motor speed, variations in marker contact, variations in the a/d oscillator frequency and variations in the sampling phase with respect to the profile centers has the effect of causing profiles to appear displaced. This displacement may be additive over the entire scan, it may be expansive over reasonable portions of the scan, for instance between markers, or it may be very local. The size of possible displacements diminish the more local the displacement.

The data available at this point in the processing cycle might now be best described in the power spectrum sense. Noiseless data would have energy content exactly matching the Fourier transform of the diffused profile (eg. Figure 5, p. 364, Refr. 4). The information is concentrated at low frequencies while noise content of the data is seen (Figure 2) to be approximately constant. Bandpass filtering will at least diminish the high frequency noise.

If time or position series data is expressed as the Fourier transform of its spectral content, then

$$F(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} G(\omega) e^{i\omega x} d\omega$$

If this data is twice differentiated it is seen,

$$\frac{d^2 F(x)}{dx^2} = \frac{-1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \omega^2 G(\omega) e^{-\omega x} d\omega$$

that the high frequency components are amplified by ω^2 . Compare for example figure 4a with figure 4b. That there is noise in the computed second differences is apparent in figure 4b. This noise is removed by the application of numerical filtering and yields a smooth second difference (figure 5a).

A definition of resolution as it applies here may best be given as "elementary profiles which are superimposed in a signal are considered resolved when there is a maximum in the data for each such elementary profile." When the separation of elementary profiles is such that the above definition is satisfied a simple algorithm may be constructed, programmed and effectively executed on the computer to select emission lines by searching for maxima.

It is shown (Appendix I) that differentiating an original profile produces another profile which, when scaled and inverted, possesses an intrinsic width which is 0.55σ at the same height that σ was computed in the original profile. This should produce an increase in resolution of 1.8.

It is not obvious that the noise content of the data has been adequately reduced by averaging if the only criterion is a comparison of figures 1 and 4a. That the high frequency energy is amplified by ω^2 when the second differences are computed is implicit when figure 4b is compared to figure 4a. When the problem of constructing a simple algorithm for the detecting of maxima in either the original profile or the computed second differences is considered, it becomes obvious that unless these

functions are very smooth the algorithm will have to do more than seek simple maxima. Since the only information of any real interest is the profile position and the peak counting rate, or relative intensity, the algorithm should not concern itself with more than the maximum unique to the simple profile it is detecting.

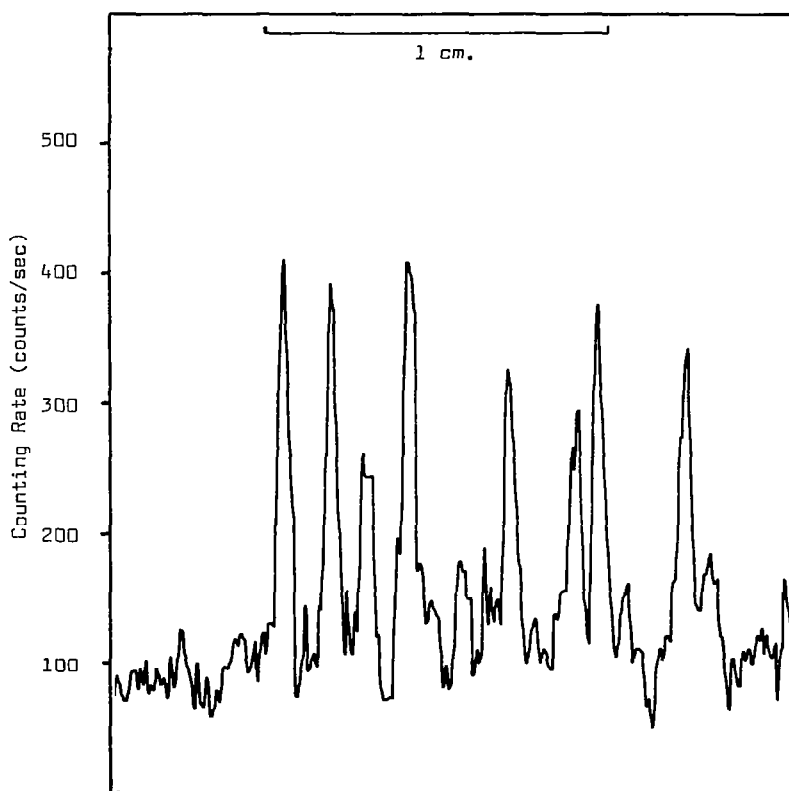


Figure 1
Sample input data after patching one point spikes
greater than 50 cps. and flagged for gaps greater
than 0.02 cm.

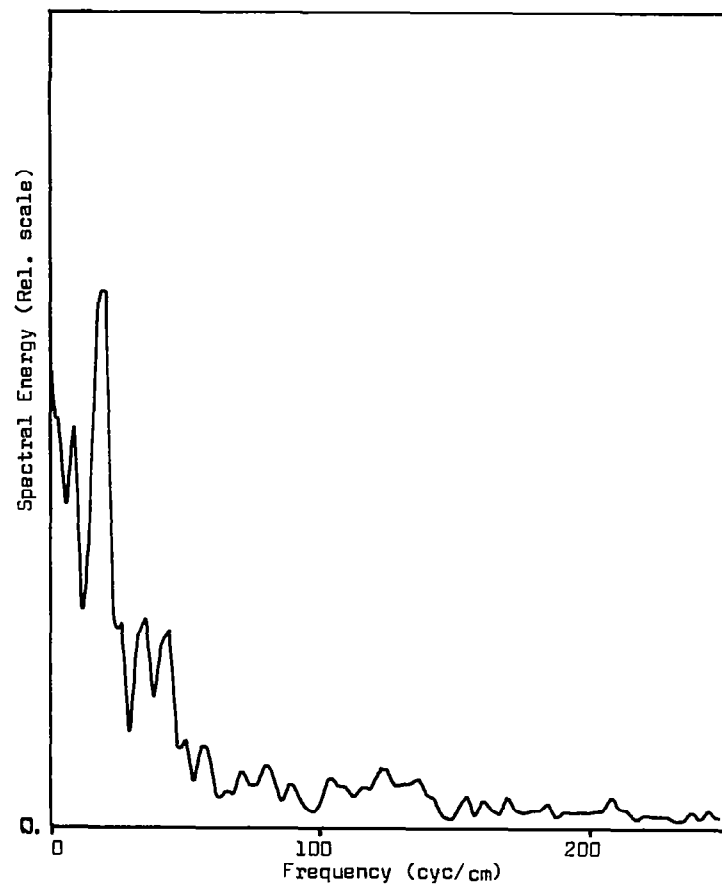


Figure 2
Computed power spectrum for data in Figure 1.

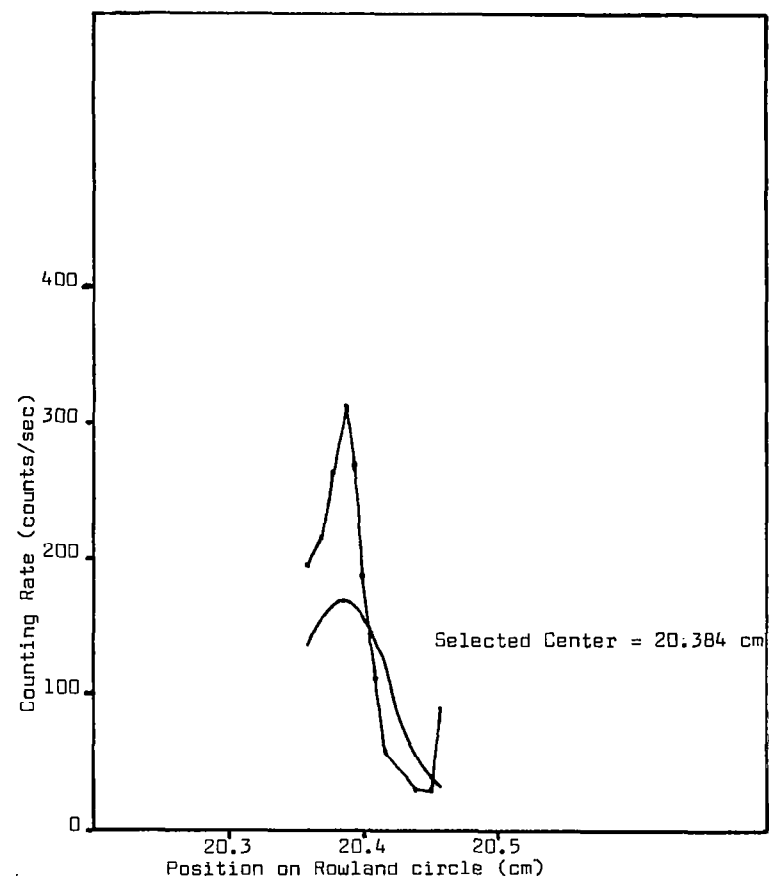


Figure 3
Sample minimum variance fit. The Gaussian is fit to the patched data to provide a reference for nonlinear averaging.

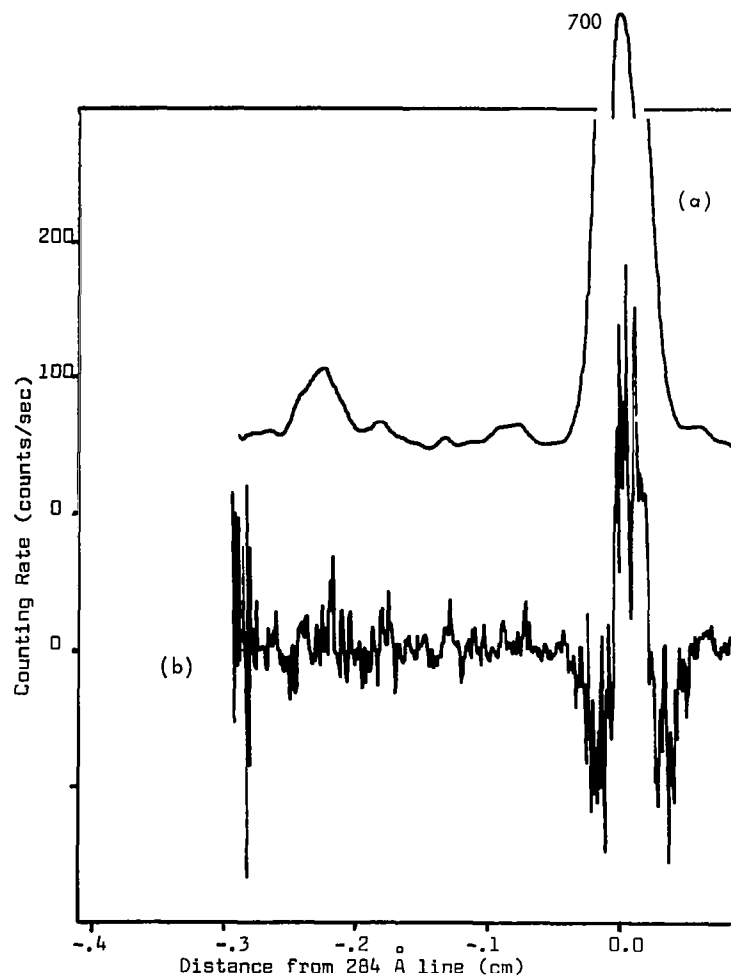


Figure 4
A sample averaged profile (the 284 Å line). a) The averaged profile; b) The computed second difference before filtering.

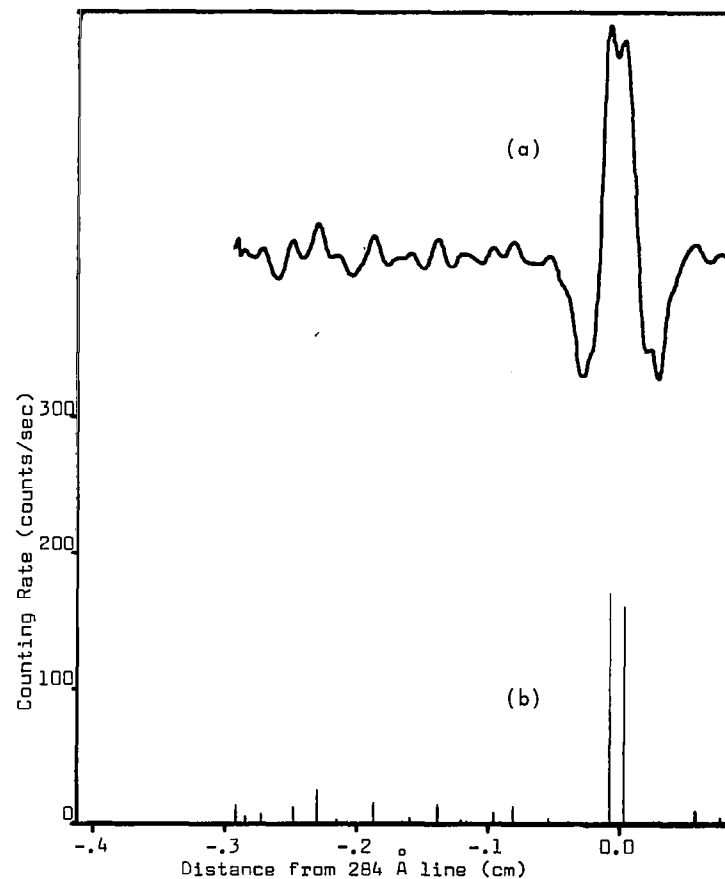


Figure 5
Smoothed second differences and line selection. a) The data in Figure 4b after numerical filtering. b) Lines selected by the program, compare Figure 4a.

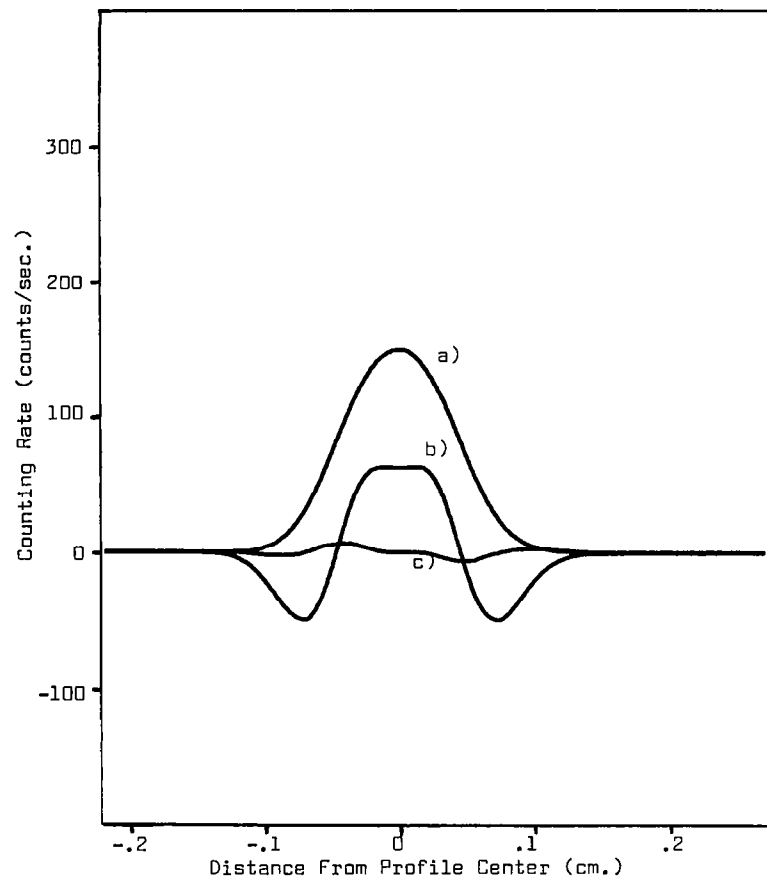


Figure 6
Theoretical analysis of a Gaussian composite consisting of two simple profiles with peak values of 100, half widths of 0.015 cm. and separated by 0.025 cm. a) the composite y . b) $\Delta^2 y$. c) $\Delta^3 y$.

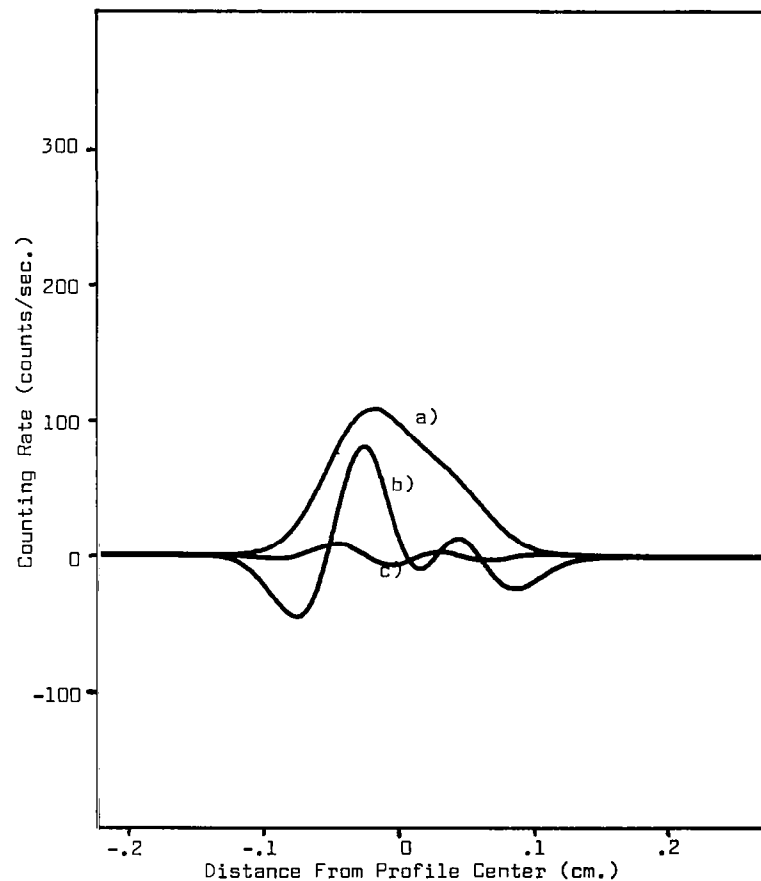


Figure 7
Theoretical analysis of a Gaussian composite consisting of two simple profiles with peak values of 100 and 50 each, half widths of 0.015 cm. and separated by 0.025 cm. a) the composite y . b) $\Delta^2 y$. c) $\Delta^3 y$.

COMPUTATIONAL APPROACH

The computational approach was selected to perform the following important functions:

- Qualify the data
- Locate references
- Average the data
- Compute second differences
- Filter numerically
- Select emission lines
- Compute confidence

Three types of error may occur in the data. The first, which must be eliminated by observation, are data fadeouts. These fadeouts occur consistently after sunrise and before sunset and occasionally at other times. Not infrequently counting rates appear in the data which are significantly different than the mean counting rate of its neighbors. These divergences are usually limited to one data value and thus are called one point spikes. These spikes if their least side exceeds 30 counts per second are eliminated and an average computed from its two neighbors is substituted. Gaps in the data which arise from markers or a digitization technique of skipping noisy analog data or from occasional random errors are detected and flagged by setting the Y value of the first data point at the beginning of the gap to a negative value. This patching and flagging is performed by subprogram D328. An example of patched data may be seen in Figure 1. Unfortunately no data gaps occurred to demonstrate flagging.

References for nonlinear averaging are located in the data by first estimating the position of the desired reference emission line, second letting the computer perform a least squares fit about this position over a suitable data interval. An example of such a fit may be seen

in Figure 3. That a correct center was selected is obvious in the figure. That the peak counting rate of the fit and the width of the fit seem different than the data is only of passing interest. The center position was the sought for information. A more careful selection would have permitted an improved fit which would have yielded the same center.

The average is accumulated as the data is located on the input tapes. The position reference is adjusted or rescaled as follows. A psuedo x-value is computed from the index i for the position to be averaged,

$$U = (i-1) (dx/di) + R_0$$

where dx/di is the step size in the averaged data. R_0 is the base or zeroth reference position. Next, the X_p position in the data is computed, this value normally lies between two input data pairs.

$$X_p = X \text{ Scale } (U - X_{Ri}) + X_{Ri}$$

where X_{Ri} is the next lower reference and $X \text{ Scale}$ is the appropriate scale factor computed when the local references were found. Finally, the interpolated counting rate at the adjusted position is computed by

$$Y_p = \frac{X_p - X_i}{X_{i+1} - X_i} (Y_{i+1} - Y_i) + Y_i$$

Here the subscript i refers to the neighboring input data points.

The observable profile width is sharpened by second differencing (see figures 6 and 7). Also, compare the 284 Å line in figure 4a and 5a. Second differences are defined and computed as

$$\Delta^2 Y = -\frac{1}{D^2} (Y_{i+1} - 2Y_i + Y_{i-1})$$

The second differences which are useless in raw form due to the w^2 noise amplification must be filtered numerically (see page 9 and figure 4b). The filter selected in this work is the first positive lobe of $\sin x/x$ which may be

adjusted by varying FA and FB (see subprogram D203).
 If it is desired that the filter have a response of 1.0
 from zero to FB, set FA = 0.0 and set,

$$FB = 1/2W$$

where W is twice the standard deviation of the original
 profiles.

The filtering algorithm used is actually,

$$\bar{f}(i) = f(i)*W(LF) + \sum_{k=2}^{NPF} (f(i-(k-1)) + f(i+(k-1))*W(LF+k-1))$$

where NPF is the number of point in half the filter W
 which is stored in memory starting at LF. The f(i)
 may be any data vector, here it is $\Delta^2 y$.

If the second differences have been optimally
 filtered each original profile which is separable by
 the current definition of resolution (see page 10) will
 be represented by a maximum value in these second
 differences. If FB was too high noise or some "ringing"
 may persist and an unreasonable number of lines will be
 selected. If FB is selected too low the profiles will
 be diffused with simultaneous degradation of resolution.

The particular algorithm used for selecting lines is
 rather simple. Maxima are sought in the smoothed second
 differences. It may be required that these maxima be
 at least greater than some value, which is also an input
 parameter (see D203). For the results presented herewith
 this parameter was set to zero so that all maxima would
 be selected.

Evaluation of mathematical confidence is made
 through numerical tests designed to detect the frequency
 of replication, confidence is thus a function of popula-
 tion density. To provide this density special computer
 runs can be made on shorter intervals of data. The

number of scans per average may be varied. The shorter analysis interval will permit many analyses, thus providing the necessary population density. Confidence for density and position may then be computed as a function of population density, number of scans, and as a function of emission line intensity.

COMPUTER PROGRAMMING

Scientific programming has at least one characteristic which justifies the adjective scientific. The programs may require "instant revision." As various algorithms are devised to carry out well defined computations, such as numerical filtering and more often the sine, exponential, etc., they should be relegated to standard computer libraries where they may be combined for the particular project. The calling sequence and compatibility of each of these subprograms usually depends upon where it appears in the main program. If it is discovered later that it would be advisable to execute a new algorithm in another portion of the program the subprogram or its calling sequence or the main program may require considerable modification.

The approach used in this effort has been to set up a compatible data memory bank such that the main program always knows where the data begins and ends within the bank. Each subprogram may now ask the main program where the data is and be given simple instructions telling it where to put the newly computed data. The main program or executive program is called D0194 and is listed in the User Manual which may be obtained through the technical officer.

The most interesting outgrowth resulting from the development of this system is that the problem may be completely redesigned through the use of the first data card called the logic-and-flag card. The first 30 fields of this card are devoted to selecting subprograms in any sequence the user may desire. The last 10 fields enable the user to vary his input or output.

If it should ever be necessary to include additional subprograms in the system no reprogramming is necessary

if the compatibility rules are observed when designing the new subprogram.

The programming languages used are Fortran IV and MAP. Fortran IV was chosen since it is the main system on the Theoretical Division computer and offers the necessary scientific language to permit a description of the problem. MAP was used to unpack data which had been compressed onto magnetic tape with the intention of performing a complete SORT to provide better access to the input data.

Again, the obvious simplicity of this system becomes apparent when the executive program D0194 is examined briefly.

CONCLUSIONS AND RECOMMENDATIONS

It has been fortunate in this work that the diffusion function has low frequency spectral characteristics which can be separated from the major noise functions. Faster scanning, narrower entrance slits and finer gratings can follow better photoelectron detectors and more rapid data rates during digitization.

Using the 284 Å line as a standard it must be concluded that lines detected which have wider profiles must be influenced by neighbors. If these neighbors are not themselves detected their existence should at least be acknowledged.

It is felt that studies of shorter portions of the data with varied filters could yield a more optimum selection with some improvement in resolution.

It can be shown that for two equal profiles the distance between the outer lobes of $\Delta^2 Y$ is $2\sqrt{3}\sigma$ when the separation C is zero and asymptotically approaches $2(C + \sqrt{3})\sigma$ for large values of C . For small C the separation differs from the asymptotic solution and could lead to an improved discussion of resolution, noise permitting.

It is recommended that the results obtained from the use of this program be recorded to permit further study. The format should be carefully studied to provide the proper archive for later experiments and cross references with other experimentors.

Finally, it is felt the effort has been successful and continued use of the program, especially on short intervals with varied numbers of scans, will yield many useful results.

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ACKNOWLEDGEMENTS

We wish to express our confidence in the Theoretical Division computer and the Data Processing plotter for their careful preparation of all of the figures in the text with the exception of Figure 3 which was drawn by hand from listed data. We also express our admiration for the Theoretical Division Computation Facility in the large. This facility attains a high productivity for standard data processing and yet maintains the degree of flexibility necessary to permit research programming and computations.

APPENDIX

PROFILE WIDTH AND RESOLUTION.

Define Profile Width, w , to be the distance between inflection points if the profile is Gaussian, that is $w = 2\sigma$. Define resolution as that separation of two simple profiles such that the additive composite is at least flat on top.

An expression is derived from the spectrometer equation which relates a step, Δx to x and the corresponding step in wavelength, $\Delta\lambda$. Thus,

$$\Delta x = f(x)\Delta\lambda \quad (1)$$

If Δx is deduced from the data by LSF to many lines where in each case x is noted, the corresponding $\Delta\lambda$ may be computed. Some lines exhibit consistently low $\Delta\lambda$. It is felt the lines which show agreement in the low $\Delta\lambda$ are single line profiles as contrasted to composites which display wider profiles. An experimental value is thus obtained for the profile width $\Delta\lambda_e$.

Using $\Delta\lambda_e$ in equation 1 the profile width $w(x)$ in cm. is obtained as a function of x . Using $\Delta\lambda_R$ also in equation 1 as the wavelength resolution desired obtain $R(x)$ in cm. Thus,

$$w = f(x) \Delta\lambda_e \quad (2)$$

$$R = f(x) \Delta\lambda_R$$

Thence,

$$\frac{w}{R} = \frac{\Delta\lambda_e}{\Delta\lambda_R} \quad (3)$$

Expressing w and R in terms of standard deviations obtain for R , since $w = 2\sigma$,

$$R = 2\sigma \frac{\Delta\lambda_R}{\Delta\lambda_e} \quad (4)$$

For a Gaussian profile,

$$y = ae^{-x^2/2\sigma^2} \quad (5)$$

A function which depends on the second derivative but yields the same value as y when $x = 0$ is given by,

$$\Delta^2 y = -\sigma^2 \frac{d^2 y}{dx^2} = (1 - (x/\sigma)^2) y \quad (6)$$

The width of this profile such that

$$\Delta^2 y = y(\sigma) = ae^{-1/2} \quad (7)$$

is obtained by solving,

$$ae^{-1/2} = (1 - (x/\sigma)^2) ae^{-x^2/2\sigma^2} \quad (8)$$

letting $x = u\sigma$, obtain

$$1 - u^2 = e^{-(1-u^2)/2} \quad (9)$$

which is approximately satisfied by $u = 0.54$.

The profile width for the function $\Delta^2 y$ is

$$w_2 = 0.54 \sigma \quad (10)$$

and resolution should be increased by the factor $1/0.54 = 1.85$.

An algorithm defining resolution for y and $\Delta^2 y$ must be established. It must then be shown that the resolution is increased by the amount indicated in the previous development. Resolution limits must then be computed.

For a composite profile consisting of two equal single profiles whose centers are separated by $2c$,

$$y = a(e^{-(x-c)^2/2\sigma^2} + e^{-(x+c)^2/2\sigma^2}) \quad (11)$$

For resolution require $y'' = 0$, that is, that the top of the profile change from downward to upward curvature so that two peaks are observed. With x in terms of σ

$$\begin{aligned} \frac{1}{a} y' &= -(x-c)e^{-(x-c)^2/2} - (x+c)e^{-(x+c)^2/2} \\ \frac{1}{a} y'' &= ((x-c)^2 - 1)e^{-(x-c)^2/2} + ((x+c)^2 - 1)e^{-(x+c)^2/2} \end{aligned} \quad (12)$$

Expect the condition to be satisfied at the profile center, $x = 0$. Thus require,

$$2(c^2 - 1)e^{-c^2/2} = 0 \quad (13)$$

or $C = \pm 1$ standard deviation. Now to find the curvature in the $\Delta^2 y$ profile, seek y^{IV} .

$$\begin{aligned} \frac{1}{a} y^{IV} = & (3 - 6(x-c)^2 + (x-c)^4)e^{-(x-c)^2/2} \\ & + (3 - 6(x+c)^2 + (x+c)^4)e^{-(x+c)^2/2} \end{aligned} \quad (14)$$

$$\text{For } x = 0, \frac{1}{2a} y^{IV}(0) = (3 - 6c^2 + c^4)e^{-c^2/2} \quad (15)$$

which is satisfied by,

$$c = \pm(3 \pm \sqrt{6}) = \pm 0.5505 \quad (16)$$

for the closest case. Thus profiles may be detected which are 1.101σ apart using second differences. This is equivalent to an increase of $1/0.550 = 1.8165$ in resolution. From the spectrometer equation deduce,

$$\Delta\lambda = 1.736 \times \Delta x (1 - 10^{-4} x^2)^{-1/2} \quad (17)$$

For the 284 Å line the measured $x = 18.629 \text{ cm.}$ and $\Delta x = \sigma = 0.015 \text{ cm.}$ and $\Delta\lambda = 0.494 \text{ Å}$ is obtained. Thus, $\sigma = \Delta\lambda = 0.494 \text{ Å}$. Note, the width at the $\frac{1}{2}$ power point is,

$$\begin{aligned} W &= 2\sigma \sqrt{\ln 4} \\ &= 1.16 \text{ Å} \end{aligned} \quad (18)$$

The necessary line separation for resolution is $2\sigma = 0.9874 \text{ Å}$. The necessary separation for resolution by 2nd differences is $2\sigma(0.55) = 0.5431 \text{ Å}$.